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8-(4-Bromophenyl)-4,4-difluoro-1,3,5,7-tetramethyl-4-bora-3a,4a-diaza-*s*-indacene

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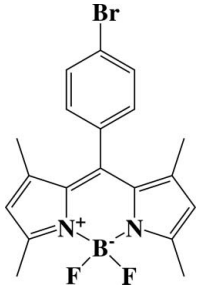
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.115; data-to-parameter ratio = 13.6.

In the molecule of the title compound, $C_{19}H_{18}BBrF_2N_2$, the bromobenzene ring is almost perpendicular to the boron–dipyrromethene (BODIPY) fused-ring fragment [dihedral angle = 78.9 (1)°].

Related literature

For related literature, see: Dost *et al.* (2006); Qin *et al.* (2005); Trieflinger *et al.* (2005); Wu *et al.* (2005).



Experimental

Crystal data

$C_{19}H_{18}BBrF_2N_2$
M_r = 403.07
Monoclinic, $P2_1/c$
a = 11.9874 (12) Å
b = 8.2874 (7) Å
c = 17.7140 (15) Å
β = 91.049 (7)°
V = 1759.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.36 mm^{-1}
T = 298 (2) K
0.62 × 0.45 × 0.10 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.323, T_{max} = 0.798
7614 measured reflections
3090 independent reflections
2354 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.115
S = 1.05
3090 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2394).

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supplementary materials

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8-(4-Bromophenyl)-4,4-difluoro-1,3,5,7-tetramethyl-4-bora-3a,4a-diaza-*s*-indacene

D.-C. Wang, C. He, J.-L. Fan, W.-W. Huang and X.-J. Peng

Comment

We are interested in the synthesis of boron-dipyrromethene (BODIPY) dyes which are well known and have attracted much attention due to their use as fluorescence labels and biomolecule sensors in recent years (Wu *et al.*, 2005; Trieflinger *et al.*, 2005; Dost *et al.*, 2006). So the investigation of their structures will be more helpful to understand their photophysical and photochemical properties profoundly (Qin *et al.*, 2005). The crystal structure of compound (I) (Fig. 1) is reported here.

As shown in Fig. 1, the BODIPY skeleton formed by three conjugated heterocyclic rings (Table 1) is almost planar, with an r.m.s. deviation of 0.0378 (3) Å; the maximum deviations from the mean plane are 0.071 (3) Å for C12 and 0.060 (3) Å for C14. The two B—N distances are almost the same, implying the usual delocalisation of the positive charge. Perhaps due to steric repulsion from the C1 and C3 methyl groups, the bormobenzene ring is strongly twisted out of the BODIPY mean plane, with a dihedral angle is 78.9 (1)°.

Experimental

Compound (I) was prepared in one-pot reaction in dichloromethane (DCM). 8 mmol (0.8 ml) 2,4-dimethyl-pyrrole and 4 mmol (735 mg) 4-bromobenzaldehyde were dissolved in 150 ml absolute DCM, a few drops of trifluoroacetic acid was added immediately under an nitrogen atmosphere. After being stirred at room temperature overnight, 200 ml DCM was evaporated, then a solution of 2,3-dichloro-5,6-dicyano-benzoquinone (4 mmol) in DCM (30 ml) was added and continue stirring for half an hour, and followed by injecting 74 mmol triethylamine (8 ml) into the dark residue, after a while, 75 mmol (12 ml) boron trifluoride ethyl ether complex was injected slowly. After stirring for about 3 hours, the solution was washed with an aqueous solution of $NaHCO_3$, the organic layer was dried over Na_2SO_4, and the solvent was evaporated by reduced pressure. Chromatography on silica column was carried out and eluted with ethyl acetate/petroleum ether (1:6 v/v) mixture. The collected red fraction was subsequently recrystallized from chloroform/hexane (1:4 v/v) to acquire 418 mg of (I) (yield 26%).

Refinement

The H atoms were placed in idealised positions (C—H = 0.93-0.96 Å) and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

Figures

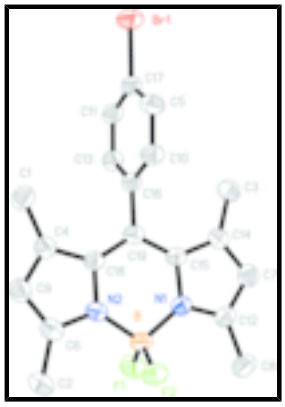


Fig. 1.

8-(4-Bromophenyl)-4,4-difluoro-1,3,5,7-tetramethyl- 4-bora-3a,4a-diaza-s-indacene

Crystal data

$C_{19}H_{18}BBrF_2N_2$	F_{000} = 816
M_r = 403.07	D_x = 1.522 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 440 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.9874 (12) Å	Cell parameters from 3357 reflections
b = 8.2874 (7) Å	θ = 2.5–32.8º
c = 17.7140 (15) Å	μ = 2.36 mm^{-1}
β = 91.049 (7)º	T = 298 (2) K
V = 1759.5 (3) Å^3	Block, dark red
Z = 4	0.62 × 0.45 × 0.10 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	3090 independent reflections
Radiation source: fine-focus sealed tube	2354 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
Detector resolution: 9.21 pixels mm^{-1}	θ_{max} = 25.0º
T = 298(2) K	θ_{min} = 2.7º
φ and ω scans	h = −14→12
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)	k = −9→9
T_{min} = 0.323, T_{max} = 0.798	l = −21→21
7614 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.115$

$S = 1.05$

3090 reflections

227 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 1.3326P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.55$ e Å^{-3}

$\Delta\rho_{min} = -0.61$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0059 (8)

Special details

Experimental. Mp.: 440-441 K;

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.641(d, 2H, Ar—H, J = 8.4 Hz), 7.171 (d, 2H, Ar—H, J = 8.4 Hz), 5.990 (s, 2H, pyrrole-H), 2.551 (s,CH_3—H, 6H), 1.141 (s, CH_3—H 6H).

^{13}C NMR ($CDCl_3$, 400 MHz): δ 156.084, 143.088, 140.196, 134.139, 132.621, 131.360, 130.017, 123.443, 121.629, 14.826.

HRMS(EI): 402.0712, calculated: 402.0714.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	−0.03359 (4)	0.71112 (6)	0.04766 (2)	0.0755 (2)
C19	0.2385 (2)	0.2985 (4)	0.27304 (17)	0.0399 (7)
C18	0.2716 (2)	0.3598 (4)	0.34286 (17)	0.0401 (7)
C17	0.0493 (3)	0.5822 (4)	0.11723 (18)	0.0478 (8)
C16	0.1705 (2)	0.4002 (4)	0.21984 (17)	0.0393 (7)
C15	0.2712 (2)	0.1449 (4)	0.24924 (17)	0.0401 (7)
C14	0.2476 (3)	0.0557 (4)	0.18261 (18)	0.0442 (8)
C13	0.0560 (3)	0.4146 (4)	0.22579 (19)	0.0464 (8)
H13A	0.0197	0.3622	0.2647	0.056*
C12	0.3683 (3)	−0.0835 (4)	0.25676 (19)	0.0462 (8)
C11	−0.0048 (3)	0.5057 (4)	0.17462 (19)	0.0489 (8)

H11A	−0.0817	0.5151	0.1790	0.059*
C10	0.2232 (3)	0.4766 (4)	0.16093 (18)	0.0468 (8)
H10A	0.3000	0.4665	0.1560	0.056*
C9	0.3057 (3)	0.5012 (4)	0.44785 (19)	0.0534 (9)
H9A	0.3077	0.5825	0.4840	0.064*
C8	0.4453 (3)	−0.2100 (5)	0.2867 (2)	0.0626 (10)
H8A	0.4735	−0.1781	0.3356	0.094*
H8B	0.5064	−0.2232	0.2530	0.094*
H8C	0.4057	−0.3102	0.2910	0.094*
C7	0.3098 (3)	−0.0832 (4)	0.18801 (19)	0.0516 (8)
H7A	0.3125	−0.1640	0.1517	0.062*
C6	0.3586 (3)	0.3521 (5)	0.45480 (19)	0.0508 (8)
C5	0.1626 (3)	0.5677 (4)	0.10936 (19)	0.0519 (9)
H5A	0.1981	0.6187	0.0697	0.062*
C4	0.2501 (3)	0.5096 (4)	0.37948 (18)	0.0463 (8)
C3	0.1662 (3)	0.0949 (5)	0.1197 (2)	0.0588 (9)
H3A	0.1691	0.0123	0.0818	0.088*
H3B	0.1852	0.1969	0.0978	0.088*
H3C	0.0921	0.1004	0.1393	0.088*
C2	0.4261 (4)	0.2875 (5)	0.5194 (2)	0.0673 (11)
H2A	0.4518	0.1810	0.5074	0.101*
H2B	0.3809	0.2830	0.5635	0.101*
H2C	0.4890	0.3567	0.5288	0.101*
C1	0.1810 (3)	0.6495 (4)	0.3533 (2)	0.0570 (9)
H1A	0.1827	0.7324	0.3911	0.086*
H1B	0.1054	0.6148	0.3446	0.086*
H1C	0.2105	0.6913	0.3072	0.086*
N2	0.3388 (2)	0.2661 (3)	0.39129 (14)	0.0422 (6)
F2	0.50032 (16)	0.0954 (3)	0.37912 (12)	0.0653 (6)
F1	0.3431 (2)	−0.0139 (3)	0.42586 (11)	0.0672 (6)
N1	0.3444 (2)	0.0526 (3)	0.29409 (14)	0.0404 (6)
B	0.3845 (3)	0.0952 (5)	0.3751 (2)	0.0455 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0897 (4)	0.0710 (3)	0.0646 (3)	0.0274 (2)	−0.0285 (2)	0.0028 (2)
C19	0.0325 (15)	0.0449 (19)	0.0424 (17)	−0.0023 (14)	0.0011 (13)	0.0054 (14)
C18	0.0355 (16)	0.0430 (18)	0.0418 (17)	0.0006 (14)	−0.0009 (13)	0.0025 (14)
C17	0.056 (2)	0.0401 (18)	0.0467 (18)	0.0091 (16)	−0.0155 (15)	−0.0060 (15)
C16	0.0382 (17)	0.0382 (17)	0.0413 (16)	0.0018 (13)	−0.0025 (13)	−0.0007 (14)
C15	0.0363 (16)	0.0418 (17)	0.0421 (17)	0.0005 (14)	−0.0015 (13)	0.0058 (15)
C14	0.0418 (17)	0.048 (2)	0.0429 (17)	−0.0043 (15)	0.0002 (14)	0.0012 (15)
C13	0.0440 (18)	0.0473 (19)	0.0480 (18)	0.0002 (15)	0.0017 (14)	0.0013 (16)
C12	0.0437 (18)	0.0439 (19)	0.0510 (19)	0.0034 (15)	0.0046 (15)	0.0030 (15)
C11	0.0398 (17)	0.050 (2)	0.057 (2)	0.0082 (15)	−0.0076 (15)	−0.0063 (17)
C10	0.0391 (17)	0.051 (2)	0.0503 (19)	0.0018 (15)	−0.0009 (14)	0.0056 (16)
C9	0.058 (2)	0.053 (2)	0.0484 (19)	−0.0030 (18)	−0.0031 (16)	−0.0070 (17)

C8	0.062 (2)	0.053 (2)	0.073 (3)	0.0149 (19)	−0.0003 (19)	0.000 (2)
C7	0.058 (2)	0.045 (2)	0.051 (2)	−0.0029 (17)	0.0021 (16)	−0.0046 (16)
C6	0.0499 (19)	0.057 (2)	0.0457 (19)	−0.0041 (17)	−0.0037 (15)	0.0013 (17)
C5	0.059 (2)	0.052 (2)	0.0447 (18)	−0.0019 (17)	−0.0055 (16)	0.0089 (16)
C4	0.0433 (18)	0.049 (2)	0.0467 (18)	−0.0012 (15)	0.0031 (14)	−0.0004 (15)
C3	0.058 (2)	0.065 (2)	0.052 (2)	−0.0001 (19)	−0.0130 (17)	−0.0078 (18)
C2	0.070 (3)	0.082 (3)	0.049 (2)	0.008 (2)	−0.0169 (19)	−0.005 (2)
C1	0.059 (2)	0.045 (2)	0.067 (2)	0.0029 (17)	−0.0035 (18)	−0.0070 (18)
N2	0.0410 (14)	0.0472 (16)	0.0381 (14)	0.0003 (12)	−0.0040 (11)	0.0037 (12)
F2	0.0450 (11)	0.0822 (16)	0.0682 (13)	0.0165 (11)	−0.0141 (9)	−0.0065 (12)
F1	0.0953 (16)	0.0553 (13)	0.0511 (12)	0.0014 (12)	0.0042 (11)	0.0145 (10)
N1	0.0377 (14)	0.0401 (15)	0.0434 (14)	0.0023 (12)	0.0014 (11)	0.0015 (12)
B	0.045 (2)	0.046 (2)	0.044 (2)	0.0046 (17)	−0.0031 (16)	0.0064 (17)

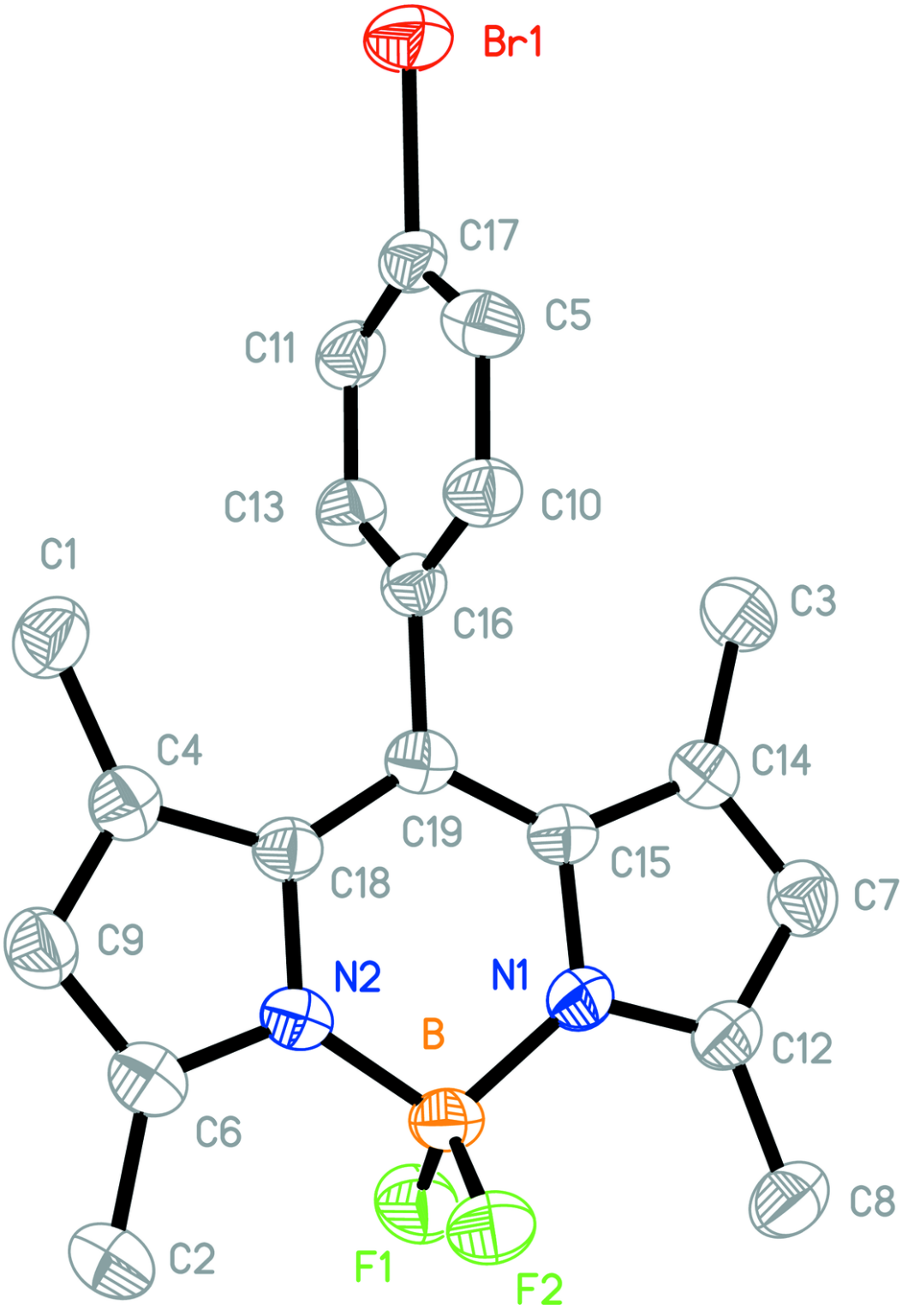
Geometric parameters (Å, °)

Br1—C17	1.898 (3)	C9—C6	1.393 (5)
C19—C18	1.388 (4)	C9—H9A	0.9300
C19—C15	1.400 (4)	C8—H8A	0.9600
C19—C16	1.495 (4)	C8—H8B	0.9600
C18—N2	1.401 (4)	C8—H8C	0.9600
C18—C4	1.426 (5)	C7—H7A	0.9300
C17—C11	1.371 (5)	C6—N2	1.349 (4)
C17—C5	1.373 (5)	C6—C2	1.489 (5)
C16—C13	1.383 (4)	C5—H5A	0.9300
C16—C10	1.384 (4)	C4—C1	1.494 (5)
C15—N1	1.400 (4)	C3—H3A	0.9600
C15—C14	1.417 (4)	C3—H3B	0.9600
C14—C7	1.374 (5)	C3—H3C	0.9600
C14—C3	1.504 (5)	C2—H2A	0.9600
C13—C11	1.377 (5)	C2—H2B	0.9600
C13—H13A	0.9300	C2—H2C	0.9600
C12—N1	1.342 (4)	C1—H1A	0.9600
C12—C7	1.394 (5)	C1—H1B	0.9600
C12—C8	1.488 (5)	C1—H1C	0.9600
C11—H11A	0.9300	B—N1	1.546 (5)
C10—C5	1.382 (4)	B—N2	1.548 (5)
C10—H10A	0.9300	B—F1	1.374 (4)
C9—C4	1.373 (5)	B—F2	1.388 (4)
C18—C19—C15	121.6 (3)	C12—C7—H7A	125.5
C18—C19—C16	119.9 (3)	N2—C6—C9	108.8 (3)
C15—C19—C16	118.4 (3)	N2—C6—C2	122.4 (3)
C19—C18—N2	119.6 (3)	C9—C6—C2	128.9 (3)
C19—C18—C4	132.3 (3)	C17—C5—C10	119.4 (3)
N2—C18—C4	108.1 (3)	C17—C5—H5A	120.3
C11—C17—C5	121.1 (3)	C10—C5—H5A	120.3
C11—C17—Br1	119.5 (3)	C9—C4—C18	105.5 (3)
C5—C17—Br1	119.4 (3)	C9—C4—C1	124.8 (3)
C13—C16—C10	119.1 (3)	C18—C4—C1	129.6 (3)

C13—C16—C19	122.1 (3)	C14—C3—H3A	109.5
C10—C16—C19	118.8 (3)	C14—C3—H3B	109.5
N1—C15—C19	120.1 (3)	H3A—C3—H3B	109.5
N1—C15—C14	107.5 (3)	C14—C3—H3C	109.5
C19—C15—C14	132.3 (3)	H3A—C3—H3C	109.5
C7—C14—C15	106.2 (3)	H3B—C3—H3C	109.5
C7—C14—C3	125.2 (3)	C6—C2—H2A	109.5
C15—C14—C3	128.5 (3)	C6—C2—H2B	109.5
C11—C13—C16	120.7 (3)	H2A—C2—H2B	109.5
C11—C13—H13A	119.7	C6—C2—H2C	109.5
C16—C13—H13A	119.7	H2A—C2—H2C	109.5
N1—C12—C7	108.7 (3)	H2B—C2—H2C	109.5
N1—C12—C8	123.6 (3)	C4—C1—H1A	109.5
C7—C12—C8	127.7 (3)	C4—C1—H1B	109.5
C17—C11—C13	119.3 (3)	H1A—C1—H1B	109.5
C17—C11—H11A	120.3	C4—C1—H1C	109.5
C13—C11—H11A	120.3	H1A—C1—H1C	109.5
C5—C10—C16	120.4 (3)	H1B—C1—H1C	109.5
C5—C10—H10A	119.8	C6—N2—C18	108.0 (3)
C16—C10—H10A	119.8	C6—N2—B	125.5 (3)
C4—C9—C6	109.6 (3)	C18—N2—B	126.6 (3)
C4—C9—H9A	125.2	C12—N1—C15	108.5 (3)
C6—C9—H9A	125.2	C12—N1—B	125.7 (3)
C12—C8—H8A	109.5	C15—N1—B	125.7 (3)
C12—C8—H8B	109.5	F1—B—F2	109.9 (3)
H8A—C8—H8B	109.5	F1—B—N1	110.3 (3)
C12—C8—H8C	109.5	F2—B—N1	110.0 (3)
H8A—C8—H8C	109.5	F1—B—N2	110.3 (3)
H8B—C8—H8C	109.5	F2—B—N2	110.3 (3)
C14—C7—C12	109.0 (3)	N1—B—N2	106.0 (3)
C14—C7—H7A	125.5		
C15—C19—C18—N2	−0.5 (4)	C6—C9—C4—C1	178.0 (3)
C16—C19—C18—N2	−177.7 (3)	C19—C18—C4—C9	−179.8 (3)
C15—C19—C18—C4	179.9 (3)	N2—C18—C4—C9	0.6 (4)
C16—C19—C18—C4	2.7 (5)	C19—C18—C4—C1	1.4 (6)
C18—C19—C16—C13	−82.5 (4)	N2—C18—C4—C1	−178.2 (3)
C15—C19—C16—C13	100.2 (4)	C9—C6—N2—C18	−0.4 (4)
C18—C19—C16—C10	100.4 (4)	C2—C6—N2—C18	178.9 (3)
C15—C19—C16—C10	−76.9 (4)	C9—C6—N2—B	178.6 (3)
C18—C19—C15—N1	−3.8 (4)	C2—C6—N2—B	−2.0 (5)
C16—C19—C15—N1	173.4 (3)	C19—C18—N2—C6	−179.8 (3)
C18—C19—C15—C14	178.8 (3)	C4—C18—N2—C6	−0.1 (3)
C16—C19—C15—C14	−3.9 (5)	C19—C18—N2—B	1.2 (4)
N1—C15—C14—C7	−2.2 (3)	C4—C18—N2—B	−179.1 (3)
C19—C15—C14—C7	175.4 (3)	C7—C12—N1—C15	−1.0 (4)
N1—C15—C14—C3	174.1 (3)	C8—C12—N1—C15	179.0 (3)
C19—C15—C14—C3	−8.3 (6)	C7—C12—N1—B	175.2 (3)
C10—C16—C13—C11	−1.1 (5)	C8—C12—N1—B	−4.7 (5)
C19—C16—C13—C11	−178.2 (3)	C19—C15—N1—C12	−175.9 (3)

C5—C17—C11—C13	0.9 (5)	C14—C15—N1—C12	2.0 (3)
Br1—C17—C11—C13	−178.8 (2)	C19—C15—N1—B	7.8 (4)
C16—C13—C11—C17	0.2 (5)	C14—C15—N1—B	−174.2 (3)
C13—C16—C10—C5	0.9 (5)	C12—N1—B—F1	−62.6 (4)
C19—C16—C10—C5	178.1 (3)	C15—N1—B—F1	113.0 (3)
C15—C14—C7—C12	1.6 (4)	C12—N1—B—F2	58.8 (4)
C3—C14—C7—C12	−174.9 (3)	C15—N1—B—F2	−125.6 (3)
N1—C12—C7—C14	−0.4 (4)	C12—N1—B—N2	178.0 (3)
C8—C12—C7—C14	179.6 (3)	C15—N1—B—N2	−6.4 (4)
C4—C9—C6—N2	0.8 (4)	C6—N2—B—F1	63.6 (4)
C4—C9—C6—C2	−178.5 (4)	C18—N2—B—F1	−117.5 (3)
C11—C17—C5—C10	−1.1 (5)	C6—N2—B—F2	−58.0 (4)
Br1—C17—C5—C10	178.7 (3)	C18—N2—B—F2	120.9 (3)
C16—C10—C5—C17	0.2 (5)	C6—N2—B—N1	−177.0 (3)
C6—C9—C4—C18	−0.8 (4)	C18—N2—B—N1	1.9 (4)

Fig. 1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